Intermolecular Potential Parameters Research of HFC Refrigerants

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In the past few years, our group done much experimental research on HFC refrigerants and measured many thermodynamic & transport properties (including P*V*Tx, sound speed, viscosity, conductivity) with high accuracy. Compared with experiment research, we just do a little research in computer simulations of the refrigerants. Our group plans to carry out computer simulation of viscosity of HFC refrigerants, but we found that the intermolecular potential parameters of HFC refrigerants are deficient. In this paper, we have determined the intermolecular potential (including square well, Lennard-Jones, Kihara, Stockmayer) parameters from P*V*Tx and sound speed data for pentafluoroethane (HFC125), 1,1,1-trifluoroethane (HFC143a), 1,1-difluoroethane (HFC152a). The experimental data used was carefully selected from many references. After we get the intermolecular potential parameters, we use it to calculate the second virial coefficient and third virial coefficient. The second virial coefficient calculated with the potential parameters determined from P*V*T*x* data is consistent with that calculated from sound speed. We think the result is acceptable. As we know, transport properties one difficult to determinate by experimental methods with high accuracy. In the paper end, we use method of molecular dynamics to research the viscosity of HFC refrigerants. The results are not good enough now, but we think it is apromising method to study the viscosity of refrigerants.